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Lower Bounds on the Ground State Entropy of the Potts Antiferromagnet on Slabs of the Simple Cubic Lattice

Robert Shrock and Yan Xu
C. N. Yang Institute for Theoretical Physics
State University of New York
Stony Brook, NY 11794

We calculate rigorous lower bounds for the ground state degeneracy per site, W, of the q-state Potts antiferromagnet on slabs of the simple cubic lattice that are infinite in two directions and finite in the third and that thus interpolate between the square (sq) and simple cubic (sc) lattices. We give a comparison with large-q series expansions for the sq and sc lattices and also present numerical comparisons.

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I. INTRODUCTION

Nonzero ground state entropy (per lattice site), $S_0 \neq 0$, is an important subject in statistical mechanics, as an exception to the third law of thermodynamics and a phenomenon involving large disorder even at zero temperature. Since $S_0 = k_B \ln W$, where $W = \lim_{n\to\infty} W_{tot.}^{1/n}$ and n denotes the number of lattice sites, $S_0 \neq 0$ is equivalent to $W > 1$, i.e., a total ground state degeneracy $W_{tot.}$ that grows exponentially rapidly as a function of n. One physical example is provided by H_2O ice, for which the residual entropy per site (at 1 atm. pressure) is measured to be $S_0 = (0.41 \pm 0.03)k_B$, or equivalently, $W = 1.51 \pm 0.05$ [1]-[3]. A salient property of ice is that the ground state entropy occurs without frustration; i.e., each of the ground state configurations of the hydrogen atoms on the bonds between oxygen atoms minimizes the internal energy of the crystal [4].

A model that also exhibits ground state entropy without frustration and hence provides a useful framework in which to study the properties of this phenomenon is the q-state Potts antiferromagnet [5]-[7] on a given lattice Λ or, more generally, a graph G, for sufficiently large q. Consider a graph $G = (V, E)$, defined by its vertex (site) and edge (bond) sets V and E. Denote the cardinalities of these sets as $n(G) = |V| \equiv n$ and $e(G) = |E|$, and let $\{G\} \equiv \lim_{n(G)\to\infty} G$. An important connection with graph theory is the fact that the zero-temperature partition function of the q-state Potts antiferromagnet on the graph G satisfies $Z(G, q, T = 0) = P(G, q)$, where $P(G, q)$ is the chromatic polynomial expressing the number of ways of coloring the vertices of G with q colors such that no two adjacent vertices have the same color (called a proper q-coloring of G) [8, 9]. Thus,

$$W(\{G\}, q) = \lim_{n\to\infty} P(G, q)^{1/n} \ . \tag{1.1}$$

In general, for certain special values of q, denoted q_s, one has the following noncommutativity of limits [10]

$$\lim_{n\to\infty} \lim_{q\to q_s} P(G, q)^{1/n} \neq \lim_{q\to q_s} \lim_{n\to\infty} P(G, q)^{1/n} \ , \tag{1.2}$$

and hence it is necessary to specify which order of limits that one takes in defining $W(\{G\}, q)$. Here by $W(\{G\}, q)$ we mean the function obtained by setting q to the given value first and then taking $n \to \infty$. For the $n \to \infty$ limit of a bipartite graph $G_{bip.}$, an elementary lower bound is $W(\{G_{bip.}\}, q) \geq \sqrt{q-1}$, so that for $q > 2$, the Potts antiferromagnet has a nonzero ground state entropy on such a lattice. A better lower bound for the square lattice is $W(sq, q) \geq (q^2-3q+3)/(q-1)$ [11]. In previous work [12]-[15] one of us and Tsai derived lower and upper bounds on W for a variety of different two-dimensional lattices. It was found that these lower bounds are quite close to the actual values as determined with reasonably good accuracy from large-q series expansions and/or Monte Carlo measurements.

In the present paper we generalize these lower bounds on two-dimensional lattice graphs by deriving lower bounds on $W(\{G\}, q)$ for sections of a three-dimensional lattice, namely the simple cubic lattice, which are of infinite extent in two directions (taken to lie along the x and y axes) and finite in the third direction, z. By comparison with large-q expansions and numerical evaluations, we show how the lower bounds for the W functions for these slabs interpolate between the values for the (respective thermodynamic limits of the) square and simple cubic lattices. These bounds are of interest partly because one does not know the exact functions $W(sq, q)$ or $W(sc, q)$ for general q.

II. CALCULATIONAL METHOD

Let us consider a section (slab) of the simple cubic lattice of dimensions $L_x \times L_y \times L_z$ vertices, which we denote $sc[(L_x)_{BCx} \times (L_y)_{BCy} \times (L_z)_{BCz}]$, where the boundary conditions (BC) in each direction are indicated by the subscripts. The chromatic polynomial of this lattice will be denoted $P(sc[(L_x)_{BCx} \times (L_y)_{BCy} \times (L_z)_{BCy}], q)$. We will calculate lower bounds for $W(sc[(L_x)_{BCx} \times (L_y)_{BCy} \times (L_z)_{BCz}], q)$ in the limit $L_x \to \infty$ and $L_y \to \infty$ with L_z fixed. These are independent of the boundary conditions imposed in the directions in which the slab is of infinite extent, and hence, for brevity of nota-

tion, we will denote the limit $\lim_{L_x,\ L_y\to\infty} sc[(L_x)_{BCx} \times (L_y)_{BCy} \times (L_z)_{BCz}]$ simply as $S_{(L_z)_{BC_z}}$, where S stands for "slab". We will consider both free (F) and periodic (P) boundary conditions in the z direction, and thus slabs such as S_{3_F}, S_{3_P}, etc. For technical reasons (to get an expression involving a trace of a coloring matrix, as explained below) we will use periodic boundary conditions in the x direction. Note that the proper q-coloring constraint implies that FBC$_z$ and PBC$_z$ are equivalent if $L_z = 2$. The number of vertices for $G = sc[(L_x)_{BCx} \times (L_y)_{BCy} \times (L_z)_{BCz}]$ is $n = L_x L_y L_z$. The specific form of Eq. (1.1) for our calculation is

$$W(S_{(L_z)_{BCz}}, q) = \lim_{L_y\to\infty} \lim_{L_x\to\infty} [P(sc[(L_x)_P \times (L_y)_{BCy} \times (L_z)_{BCz}], q)]^{1/n} \ . \tag{2.1}$$

To derive a lower bound on $W(S_{(L_z)_{BC_z}}, q)$, we generalize the method of Refs. [11]-[14] from two to three dimensions. We consider two adjacent transverse slices of the slab orthogonal to the x direction, with x values x_0 and x_0+1. These are thus sections of the square lattice of dimension $L_y \times L_z$, which we denote $G_{x_0} = sq[(L_y)_{BC_y} \times (L_z)_{BC_z}]_{x_0}$ and $G_{x_0+1} = sq[(L_y)_{BC_y} \times (L_z)_{BC_z}]_{x_0+1}$. We label a particular color assignment to the vertices of G_{x_0} that is a proper q-coloring of these vertices as $C(G_{x_0})$ and similarly for G_{x_0+1}. The total number of proper q-colorings of G_{x_0} is

$$\mathcal{N} = P(G_{x_0}, q) = P(G_{x_0+1}, q) \ . \tag{2.2}$$

Now let us add the edges in the x direction that join these two adjacent transverse slices of the slab together. Among the $\mathcal{N}^2$ color configurations that yield proper q-colorings of these two separate yz transverse slices, some will continue to be proper q-colorings after we add these edges that join them in the x direction, while others will not. We define an $\mathcal{N} \times \mathcal{N}$-dimensional coloring compatibility matrix T with entries $T_{C(G_{x_0}),C(G_{x_0+1})}$ equal to (i) 1 if the color assignments $C(G_{x_0})$ and $C(G_{x_0+1})$ are proper q-colorings after the edges in the x direction have been added joining G_{x_0} and G_{x_0+1}, i.e., if the color assigned to each vertex $v(x_0, y, z)$ in G_{x_0} is different from the color assigned to the vertex $v(x_0+1, y, z)$ in G_{x_0+1}; and (ii) 0 if the color assignments $C(G_{x_0})$ and $C(G_{x_0+1})$ are not proper q-colorings after the edges in the x direction have been added, i.e., there exists some color assigned to a vertex $v(x_0, y, z)$ in G_{x_0} that is equal to a color assigned to the vertex $v(x_0+1, y, z)$ in G_{x_0+1}. Clearly, $T_{ij} = T_{ji}$. The chromatic polynomial for the slab is then given by the trace

$$P(sc[(L_x)_P \times (L_y)_{BCy} \times (L_z)_{BC_z}], q) = \mathrm{Tr}(T^{L_x}) \ . \tag{2.3}$$

Since T is a real symmetric matrix, there exists an orthogonal matrix A that diagonalizes T: $ATA^{-1} = T_{diag.}$. Let us denote the $\mathcal{N}$ eigenvalues of T as $\lambda_{T,j}$, $1 \le j \le \mathcal{N}$. Since T is a real non-negative matrix, we can apply the generalized Perron-Frobenius theorem [17, 18] to infer that T has a real maximal eigenvalue, which we denote $\lambda_{T,max}$. It follows that

$$\lim_{L_x\to\infty} [P(sc[(L_x)_P \times (L_y)_{BCy} \times (L_z)_{BC_z}], q)]^{1/L_x} = \lambda_{T,max} \ . \tag{2.4}$$

Now for the transverse slices G_{x_0} and G_{x_0+1}, denoted generically as $ts((L_z)_{BC_z})$, the chromatic polynomial has the form

$$P(G_{x_0}, q) = P(G_{x_0+1}, q) = \sum_j c_j \, (\lambda_{ts((L_z)_{BC_z}),j})^{L_y} \tag{2.5}$$

where the c_j are coefficients whose precise form is not needed here. The set of $\lambda_{ts((L_z)_{BC_z}),j}$'s is independent of the length L_y and although this set depends on BC_y, the maximal one (having the largest magnitude), $\lambda_{ts((L_z)_{BC_z}),max}$, is independent of BC_y (e.g., [16] and references therein). Hence,

$$\begin{aligned} \lim_{L_y\to\infty} [P(G_{x_0}, q)]^{1/L_y} &\equiv \lim_{L_y\to\infty} (\mathcal{N})^{1/L_y} \\ &= \lambda_{ts((L_z)_{BC_z}),max} \ . \end{aligned} \tag{2.6}$$

The two adjacent slices together with the edges in the x direction that join them constitute the graph $sc[2_F \times (L_y)_{BCy} \times (L_z)_{BC_z}]$. We denote the chromatic polynomial for this section (tube) of the sc lattice as $P(sc[2_F \times (L_y)_{BCy} \times (L_z)_{BC_z}], q)$ (which is equal to $P(sc[2_P \times (L_y)_{BCy} \times (L_z)_{BC_z}], q)$ because of the proper q-coloring condition). This has the form

$$\begin{aligned} & P(sc[2_F \times (L_y)_{BCy} \times (L_z)_{BC_z}], q) \\ &= \sum_j c'_j \, (\lambda_{tube((L_z)_{BC_z}),j})^{L_y} \end{aligned} \tag{2.7}$$

where c'_j are coefficients analogous to those in (2.5). Therefore,

$$\begin{aligned} \lim_{L_y\to\infty} \quad & [P(sc[2_F \times (L_y)_{BCy} \times (L_z)_{BC_z}], q)]^{1/L_y} = \\ &= \lambda_{tube((L_z)_{BC_z}),max} \ . \end{aligned} \tag{2.8}$$

Now let us denote the column sum (CS)

$$CS_j(T) = \sum_{i=1}^{\mathcal{N}} T_{ij} \ , \tag{2.9}$$

which is equal to the row sum $\sum_{j=1}^{\mathcal{N}} T_{ij}$, since $T^T = T$. We also define the sum of all entries (SE) of T as

$$SE(T) = \sum_{i,j=1}^{\mathcal{N}} T_{ij} \ . \tag{2.10}$$

Note that $SE(T)/\mathcal{N}$ is the average row (= column) sum. Next, we observe that

$$SE(T) = P(sc[2_F \times (L_y)_{BCy} \times (L_z)_{BC_z}], q) \ . \tag{2.11}$$

To obtain our lower bound, we then use the $r = 1$ special case of the theorem that for a non-negative symmetric matrix T and $r \in \mathbb{N}_+$ [19]

$$\lambda_{max}(T) \ge \left[\frac{SE(T^r)}{\mathcal{N}}\right]^{1/r} \ . \tag{2.12}$$

The lower bound is then

$$W(S_{(L_z)_{BC_z}}, q) \ge W(S_{(L_z)_{BC_z}}, q)_\ell \tag{2.13}$$

where

$$\begin{aligned} W(S_{(L_z)_{BC_z}}, q)_\ell &= \lim_{L_y \to \infty} \left(\frac{SE(T)}{\mathcal{N}}\right)^{1/(L_y L_z)} \\ &= \lim_{L_y \to \infty} \left[\frac{P(sc[2_F \times (L_y)_{BCy} \times (L_z)_{BC_z}], q)}{P(sq[(L_y)_{BCy} \times (L_z)_{BC_z}], q)}\right]^{1/(L_y L_z)} \\ &= \left[\frac{\lambda_{tube((L_z)_{BC_z}),max}}{\lambda_{ts((L_z)_{BC_z}),max}}\right]^{1/L_z} \ . \end{aligned} \tag{2.14}$$

III. RESULTS FOR SLAB OF THICKNESS $L_z = 2$ WITH FBC$_z$

We now evaluate our general lower bound in Eqs. (2.13) and (2.14) for a slab of the simple cubic lattice with thickness $L_z = 2$ and FBC$_z$, denoted S_{2_F}. In this case the transverse slice is the graph $sq[2_F \times (L_y)_{BCy}]$. For FBC$_y$, an elementary calculation yields

$$P(sq[2_F \times (L_y)_F], q) = q(q-1)(q^2 - 3q + 3)^{L_y - 1} \tag{3.1}$$

with a single $\lambda_{ts(2_F)} = \lambda_{ts(2_P)} \equiv \lambda_{ts(2)}$, and this is also the maximal λ for PBC$_y$ [10, 20], so that

$$\lambda_{ts(2),max} = q^2 - 3q + 3 \ . \tag{3.2}$$

We next use the calculation of

$$\begin{aligned} P(sc[2_F \times (L_y)_F \times 2_F], q) &= P(sc[2_F \times 2_F \times (L_y)_F], q) \\ &= P(sq[4_P \times (L_y)_F], q) \end{aligned} \tag{3.3}$$

in Ref. [34] (where each of the 2_F BC's is equivalent to 2_P), from which we calculate the maximal $\lambda_{tube(2),max}$ to be

$$\lambda_{tube(2),max} = \frac{1}{2}\left[q^4 - 8q^3 + 29q^2 - 55q + 46 + \sqrt{R_{22}}\,\right] \tag{3.4}$$

where

$$\begin{aligned} R_{22} &= q^8 - 16q^7 + 118q^6 - 526q^5 + 1569q^4 \\ &- 3250q^3 + 4617q^2 - 4136q + 1776 \ . \end{aligned} \tag{3.5}$$

We then substitute these results for $\lambda_{ts(2),max}$ and $\lambda_{tube(2),max}$ into the $L_z = 2$ special case of (2.14) to obtain $W(S_2, q)_\ell$, and thus the resultant lower bound on $W(S_{2_F}, q) = W(S_{2_P}, q) \equiv W(S_2, q)$: $W(S_2, q) \ge W(S_2, q)_\ell$.

IV. COMPARISON WITH LARGE-q SERIES EXPANSIONS

One way to elucidate how this lower bound $W(S_2, q)_\ell$ compares with the exact $W(sq, q)$ and $W(sc, q)$ is to compare the large-q series expansions for these three functions. For this purpose, it is first appropriate to give some relevant background on large-q series expansions for $W(\{G\}, q)$ functions. Since there are q^n possible colorings of the vertices of an n-vertex graph G with q colors

if no conditions are imposed, an obvious upper bound on the number of proper q-colorings of the vertices of G is $P(G,q) \le q^n$. This yields the corresponding upper bound $W(\{G\},q) < q$. Hence, it is natural to define a reduced function that has a finite limit as $q \to \infty$,

$$W_r(\{G\},q) = q^{-1} W(\{G\},q) \ . \tag{4.1}$$

For a lattice or, more generally, a graph whose vertices have bounded degree, $W_r(\{G\},q)$ is analytic about $1/q = 0$. ($W_r(\{G\},q)$ is non-analytic at $1/q = 0$ for certain families of graphs that contain one or more vertices with unbounded degree as $n \to \infty$, although the presence of a vertex with unbounded degree in this limit does not necessarily imply non-analyticity of $W_r(\{G\},q)$ at $1/q = 0$ [21, 22].) It is conventional to express the large-q Taylor series for a function that has some factors removed from W_r, since this function yields a simpler expansion. A chromatic polynomial has the general form

$$P(G,q) = \sum_{j=0}^{n-k(G)} (-1)^j a_{n-j} q^{n-j} \ , \tag{4.2}$$

where the $a_{n-j} > 0$ and $k(G)$ is the number of connected components of G (taken here to be $k(G) = 1$ without loss of generality). One has $a_n = 1$, $a_{n-1} = e(G)$, and, provided that the girth $g(G) > 3$ [23], as is the case here, $a_{n-2} = \binom{e(G)}{2}$. A κ-regular graph is a graph such that each vertex has degree (coordination number) κ. For a κ-regular graph, $e(G) = \kappa n/2$. The coefficients of the three terms of highest degree in q in $P(G,q)$ for a κ-regular graph are precisely the terms that would result from the expansion of $[q(1-q^{-1})^{\kappa/2}]^n$. Hence, for a κ-regular graph or lattice, one usually displays the large-q series expansions for the reduced function

$$\overline{W}(\Lambda,q) = \frac{W(\Lambda,q)}{q(1-q^{-1})^{\kappa/2}} \ . \tag{4.3}$$

The large-q Taylor series for this function can be written in the form

$$\overline{W}(\Lambda,q) = 1 + \sum_{j=1}^{\infty} w_{\Lambda,j} y^j \ , \tag{4.4}$$

where

$$y = \frac{1}{q-1} \ . \tag{4.5}$$

The two results that we shall need here are the large-q (i.e., small-y) Taylor series for $\overline{W}(sq,q)$ and $\overline{W}(sc,q)$. The large-q series for $\overline{W}(sq,q)$ was calculated to successively higher orders in [24]-[28]. Here we only quote the terms to $O(y^{11})$:

$$\begin{aligned}\overline{W}(sq,q) &= 1 + y^3 + y^7 + 3y^8 + 4y^9 + 3y^{10} \\ &+ 3y^{11} + O(y^{12}) \ . \end{aligned} \tag{4.6}$$

As noted above, lower bounds on $W(\Lambda,q)$ obtained from the inequality (2.12) for two-dimensional lattices Λ were found to be quite close to the actual values of the respective $W(\Lambda,q)$ for a large range of values of q. This can be understood for large values of q from the fact that they coincide with the large-q expansions to many orders, and the agreement actually extends to values of q only moderately above $q = 2$. For example, the lower bound on $W(sq,q)$ in [11] is equivalent to $\overline{W}(sq,q) \ge (1+y^3)$. This agrees with the small-y series up to order $O(y^6)$, as is evident from comparison with Eq. (4.6). This lower bound also agrees quite closely with the value of $W(sq,q)$ determined by Monte Carlo simulations in [10, 12, 13] (see Table 1 of [10] and Table 1 of [12]). We include this comparison here in Table I. For our purposes, it is sufficient to quote the results from Ref. [10] only to three significant figures. Since we are using large-q series for this comparison, we list the results in Table I for a set of values $q \ge 4$. As another example, the lower bound obtained for the honeycomb lattice in Ref. [13], $\overline{W}(hc,q) \ge (1+y^5)^{1/2}$, agreed with the small-$y$ series for $\overline{W}(hc,q)$ to $O(y^{10})$. Thus, it was found that for all of the cases studied, $W(\Lambda,q)_\ell$ provides not only a lower bound on $W(\Lambda,q)$, but a rather good approximation to the latter function. It is thus reasonable to expect that this will also be true for the lower bounds $W(S_{(L_z)_{BC_z}},q)_\ell$ for the slabs S_{L_z} of the simple cubic lattice considered here, of infinite extent in the x and y directions and of thickness L_z in the z direction.

From ingredients given in Ref. [25], we have calculated a large-q expansion of the $\overline{W}(sc,q)$ for the simple cubic (sc) lattice and obtain

$$\overline{W}(sc,q) = 1 + 3y^3 + 22y^5 + 31y^6 + O(y^7) \ . \tag{4.7}$$

In Table I we list the corresponding values of $W(sc,q)$ obtained from this large-q series, denoted $W(sc,q)_{ser.}$, for $q \ge 4$. We also list estimates of $W(sc,q)$, denoted $W(sc,q)_{MC}$, for $4 \le q \le 6$ from the Monte Carlo calculations in Ref. [29]. One sees that the approximate values obtained from the large-q series are close to the estimates from Monte Carlo simulations even for q values as low as $q = 4$.

The coordination number for the S_{2_F} slab of the simple cubic lattice (of infinite extent in the x and y directions) is $\kappa(S_{2_F}) = 5$. We thus analyze the reduced function $\overline{W}(S_2,q)_\ell = W(S_2,q)_\ell/[q(1-q^{-1})^{5/2}]$. This has the large-$q$ (small-y) expansion

$$\overline{W}(S_2,q)_\ell = 1 + 2y^3 + 2y^5 + 9y^6 + O(y^7) \ . \tag{4.8}$$

As this shows, $\overline{W}(S_2,q)_\ell$ provides an interpolation between $\overline{W}(sq,q)$ and $\overline{W}(sc,q)$; for example, the coefficient of the y^3 term is 1 for $\Lambda = sq$, 2 for $\Lambda = S_2$, and 3 for $\Lambda = sc$. Furthermore, the coefficient of the y^5 term is 0 for $\Lambda = sq$, 2 for $\Lambda = S_2$, and 22 for $\Lambda = sc$. This is in agreement with the fact that the exact functions $W(S_{(L_z)_F},q)$ interpolate between $W(sc,q)$ and $W(sc,q)$ as L_z increases from 1 to ∞ [30] and the expectation,

as discussed above, that $W(S_{(L_z)_F},q)_\ell$ should be close to $W(S_{(L_z)_F},q)$.

V. RESULTS FOR SLABS OF THICKNESS $L_z = 3,\ 4$ WITH FBC$_z$

For the slab of the simple cubic lattice with thickness $L_z = 3$ and FBC$_z$, denoted S_{3_F}, the transverse slice is the graph $sq[3_F \times (L_y)_{BCy}]$. The chromatic polynomials $P(sq[3_F \times (L_y)_F],q)$, $P(sq[3_F \times (L_y)_P],q)$, and $P(sq[3_F \times (L_y)_{TP}],q)$ (where TP denotes twisted periodic, i.e., Möbius BC) were computed for arbitrary L_y in Refs. [31], [32], and [33], respectively, and the maximal λ was shown to be the same for all of these boundary conditions. For the reader's convenience, we list this $\lambda_{ts(3_F),max}$ in Eqs. (9.2) and (9.3) of the Appendix. The other input that is needed to obtain the lower bound in Eq. (2.14) is the maximal λ for the chromatic polynomial of the $sc[2_F \times 3_F \times L_y]$ tube graph, i.e., $\lambda_{tube(3_F),max}$. The relevant transfer matrix that determines the chromatic polynomial for this tube graph was given with Ref. [34]. Because it is 13×13 dimensional, one cannot solve the corresponding characteristic polynomial analytically to obtain $\lambda_{tube(3_F),max}$ for general q. However, one can calculate $\lambda_{tube(3_F),max}$ numerically, and we have done this. Combining these results with Eqs. (9.2) and (9.3), we then evaluate the lower bound $W(S_{3_F},q)_\ell$ by evaluating the $L_z = 3$ special case of (2.14).

For the slab of the simple cubic lattice with thickness $L_z = 4$ and FBC$_z$, S_{4_F}, the transverse slice is the graph $sq[4_F \times (L_y)_{BCy}]$. Here the maximal $\lambda_{ts(4_F),max}$ is the solution of the cubic equation (9.5) given in the Appendix. One also needs the maximal λ for the chromatic polynomial of the $sc[2_F \times 4_F \times L_y]$ tube graph, i.e., $\lambda_{tube(4_F),max}$. The relevant (136×136 dimensional) transfer matrix for this tube graph was calculated for Ref. [34], and we have used this to compute $\lambda_{tube(4_F),max}$ numerically. We then obtain the lower bound $W(S_{4_F},q)_\ell$ from the $L_z = 4$ special case of Eq. (2.14). The results for $W(S_{3_F},q)$ and $W(S_{4_F},q)$ are listed in Table I.

VI. RESULT FOR SLAB OF THICKNESS $L_z = 3$ WITH PBC$_z$

It is also of interest to obtain a lower bound for W for a slab with periodic boundary conditions in the z direction, since these minimize finite-volume effects. For this purpose we consider the slab of the simple cubic lattice with thickness $L_z = 3$ and PBC$_z$, S_{3_P}. In this case the transverse slice is the graph $sq[3_P \times (L_y)_{BCy}]$. For FBC$_y$ the chromatic polynomial involves only one λ, and this is also the maximal λ for PBC$_y$ and TPBC$_y$ [36], viz.,

$$\lambda_{ts(3_P),max} = q^3 - 6q^2 + 14q - 13 \ . \tag{6.1}$$

One then needs $\lambda_{tube(3_P),max}$. The relevant (4×4 dimensional) transfer matrix for this tube graph was calculated for Ref. [34], and we have used this to compute $\lambda_{tube(3_P),max}$ numerically. The results for $W(S_{3_P},q)$ are given in Table I.

VII. DISCUSSION

Since the slabs of infinite extent in the x and y directions and of finite thickness L_z geometrically interpolate between the square and simple cubic lattices, it follows that the resultant W functions for these slabs interpolate between $W(sq,q)$ and $W(sc,q)$ [30]. Given that it was shown previously that the lower bounds $W(\Lambda,q)_\ell$ obtained by the coloring matrix method are quite close to the actual values of the respective $W(\Lambda,q)$ for a number of two-dimensional lattices, this is also expected to be true for the $W(S_{(L_z)_{BC_z}},q)_\ell$ bounds. We have shown above how $W(S_2,q)_\ell$ interpolates between $W(sq,q)$ and $W(sc,q)$ via a comparison of the large-q series expansions for these three functions. Table I provides a further numerical comparison for $W(S_{3_F},q)_\ell$, $W(S_{4_F},q)$, and $W(S_{3_P},q)$ with $W(sq,q)$ and $W(sc,q)$, the latter being determined to reasonably good accuracy from large-q series expansions and, where available, Monte Carlo measurements. As noted, the lower end of the range of q values for the comparison is chosen as $q = 4$ in view of the use of large-q series.

For sections of lattices, and, more generally, graphs that are not κ-regular, one can define an effective vertex degree (coordination number) as [14]

$$\kappa_{eff} = \frac{2e(G)}{n(G)} \ . \tag{7.1}$$

For $3 \le L_z < \infty$, the slab of the simple cubic lattice (of infinite extent in the x and y directions) with FBC$_z$ is not κ-regular, but has the effective coordination number

$$\kappa_{eff}(S_{(L_z)_F}) = 2\left(3 - \frac{1}{L_z}\right) \ . \tag{7.2}$$

We observe that for the q values considered in Table I, $W(sq,q) > W(S_2,q)_\ell > W(S_{3_F},q)_\ell > W(S_{4_F},q) > W(sc,q)$. The fact that for fixed q, the exact function $W(S_{(L_z)_F},q)$ is a non-increasing function of L_z, and, for $q > 2$, a monotonically decreasing function of L_z, follows from a theorem proved in Ref. [30]. To the extent that the lower bounds $W(S_{(L_z)_F},q)_\ell$ lie close to the actual values of $W(S_{(L_z)_F},q)$, it is understandable that they also exhibit the same strict monotonicity. As was noted in Ref. [30], the reason for the monotonicity of the exact values is that the number of proper q-colorings per vertex of a lattice graph is more highly constrained as one increases the effective coordination number of the lattice section. (This is also evident in Fig. 5 of [10].) In the present case, the monotonicity can be seen as a result of

the fact that the effective coordination number increases monotonically as a function of L_z.

The use of periodic boundary conditions in the z direction minimizes finite-size effects, so that for a given L_z, $W(S_{(L_z)_P}, q)$ would be expected to be closer to $W(sc, q)$ than $W(S_{(L_z)_F}, q)$ [30]. Again, to the extent that the lower bounds are close to the actual W functions for these respective slabs, one would expect $W(S_{(L_z)_P}, q)_\ell$ to be closer than $W(S_{(L_z)_F}, q)_\ell$ to $W(sc, q)$. Our results agree with this expectation. In contrast to $W(S_{(L_z)_F}, q)$, $W(S_{(L_z)_P}, q)$ is not, in general, a non-increasing function of L_z, as was discussed in general in [30] (see Fig. 1 therein). Thus, values of $W(S_{(L_z)_P}, q)$, and hence, *a fortiori*, $W(S_{(L_z)_P}, q)_\ell$, may actually lie slightly below those for $W(sc, q)$, as is evident for the $W(S_{3_P}, q)_\ell$ entries in Table I.

VIII. CONCLUSIONS

In this paper we have calculated rigorous lower bounds for the ground state degeneracy per site W, equivalent to the ground state entropy $S_0 = k_B \ln W$, of the q-state Potts antiferromagnet on slabs of the simple cubic lattice that are infinite in two directions and finite in the third. Via comparison with large-q expansions and numerical evaluations, we have shown how the results interpolate between the square (sq) and simple cubic (sc) lattices.

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IX. APPENDIX

We note the following results on $\mathbb{E}^d$ lattices and lattice sections: $W(\Lambda_{bip.}, 2) = 1$ for any bipartite lattice; $W(sq, 3) = (4/3)^{3/2}$ [37]; and $W(\{L\}, q) = W(\{C\}, q) = q - 1$, where L_n and C_n denote the n-vertex line and circuit graphs. For the infinite-length square-lattice strip of width 2, $W(sq[2_F \times \infty], q) = W(sq[2_P \times \infty], q) = \sqrt{q^2 - 3q + 3}$, where, as in the text, the subscripts F and P denote free and periodic boundary conditions in the direction in which the strip is finite. For the infinite-length strip of the square lattice with (transverse) width 3 and free transverse boundary conditions, $sq[3_F \times \infty]$ [31–33]

$$W(sq[3_F \times \infty], q) = (\lambda_{3_F,max})^{1/3} \tag{9.1}$$

where

$$\lambda_{3_F,max} = \frac{1}{2}\left[(q-2)(q^2-3q+5) + \sqrt{R_3}\,\right] \tag{9.2}$$

with

$$R_3 = (q^2 - 5q + 7)(q^4 - 5q^3 + 11q^2 - 12q + 8) \ . \tag{9.3}$$

For the infinite-length strip of the square lattice with width 4 and free transverse boundary conditions, $sq[4_F \times \infty]$ [31, 35]

$$W(sq[4_F \times \infty], q) = (\lambda_{4_F,max})^{1/4} \tag{9.4}$$

where $\lambda_{4_F,max}$ is the largest root of the cubic equation

$$x^3 + b_{4_F,1}x^2 + b_{4_F,2}x + b_{4_F,3} = 0 \tag{9.5}$$

with

$$b_{4_F,1} = -q^4 + 7q^3 - 23q^2 + 41q - 33 \tag{9.6}$$

$$b_{4_F,2} = 2q^6 - 23q^5 + 116q^4 - 329q^3 + 553q^2 - 517q + 207 \tag{9.7}$$

and

$$\begin{aligned} b_{4_F,3} &= -q^8 + 16q^7 - 112q^6 + 449q^5 - 1130q^4 + 1829q^3 \\ &- 1858q^2 + 1084q - 279 \ . \end{aligned} \tag{9.8}$$

TABLE I: Comparison of lower bounds $W(S_{(L_z)_{BCz}}, q)_\ell$ for $(L_z)_{BCz} = 2_F = 2_P,\ 3_F,\ 4_F,\ 3_P$ with approximate values of $W(\Lambda, q)$ for the square (sq) and simple cubic (sc) lattices Λ, as determined from large-q series expansions, denoted $W(\Lambda, q)_{ser.}$ and, where available, Monte Carlo simulations, denoted $W(\Lambda, q)_{MC}$. We also list $W(sq, q)_\ell$ for reference. See text for further details.

q	$W(sq,q)_{MC}$	$W(sq,q)_{ser.}$	$W(sq,q)_\ell$	$W(S_{2_F},q)_\ell$	$W(S_{3_F},q)_\ell$	$W(S_{4_F},q)_\ell$	$W(sc,q)_{ser.}$	$W(sc,q)_{MC}$	$W(S_{3_P},q)_\ell$
4	2.34	2.34	2.33	2.13	2.07	2.04	2.06	1.9	1.78
5	3.25	3.25	3.25	2.96	2.875	2.83	2.75	2.7	2.62
6	4.20	4.20	4.20	3.87	3.765	3.71	3.58	3.6	3.51
7	5.17	5.17	5.17	4.81	4.69	4.64	4.48	–	4.43
8	6.14	6.14	6.14	5.76	5.64	5.58	5.41	–	5.37
9	7.125	7.125	7.125	6.73	6.605	6.54	6.36	–	6.325
10	8.11	8.11	8.11	7.71	7.58	7.51	7.32	–	7.29
100	–	98.0	98.0	97.5	97.4	97.3	97.0	–	97.0

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